

chain nodes :

6 8 9 16 17 18 19 20 21 22 23 24 25 26 27 37 38 40 43 ring nodes :

1 2 3 4 5 10 11 12 13 14 15 47 48 49 54 55 56 57 chain bonds :

2-6 3-8 4-9 5-37 10-38 11-46 12-40 13-52 17-18 19-20 19-21 19-22 56-62 ring bonds :

48-49 54-55 1-2 1-5 3-4 3-72 4-72 10-11 11-12 13-14 14-15 14-47 15-49 47-48 54-57 55-56 55-59 57-58 58-59

exact/norm bonds :

1-2 1-5 2-6 3-8 3-4 3-72 4-9 4-72 5-37 10-11 10-38 11-12 11-46 12-40 13-14 13-52 14-15 14-47 15-49 17-18 19-20 19-21 19-22 47-48 48-49 54-55 54-57 55-56 55-59 56-62 57-58 58-59

G1: [*1], [*2], [*3], [*4], [*5], [*6], [*7], [*8]

G2:Si, Hy, Ak, [*9]

G3: [*10-*11], [*12-*13], [*14-*15], [*16-*17]

Connectivity:

1:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS

22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 37:CLASS 38:Atom 40:CLASS

43:Atom

46:CLASS 47:Atom 48:Atom 49:Atom 52:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 62:CLASS 72:Atom

Generic attributes :

6:

Number of Hetero Atoms : 2 or more

8:

Saturation : Unsaturated

9:

Saturation : Unsaturated

38:

Number of Hetero Atoms : 2 or more

43:

Saturation : Unsaturated

52:

Saturation : Unsaturated

Element Count :

Node 6: Limited

N,N1

Node 38: Limited

N,N1

Node 52: Limited

N,N1

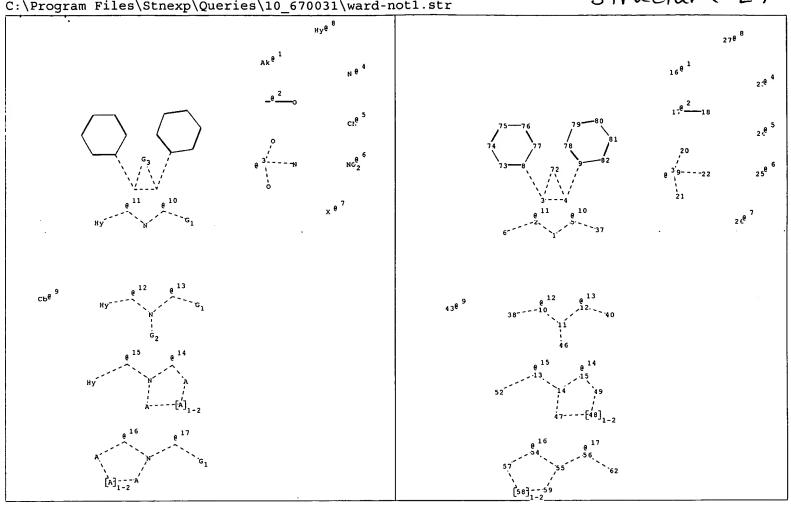
chain nodes :

G2:Si,Hy,Ak,[*9]

Connectivity:

G1: [*1], [*2], [*3], [*4], [*5], [*6], [*7], [*8]

G3: [*10-*11], [*12-*13], [*14-*15], [*16-*17]



```
27
                                                 37
                                      25
                                                                   52
   6 16
        17 18
                19 20
                        21
                           22
                               23
                                   24
                                          26
                                                     38
                                                        40
                                                            43
                                                                46
ring nodes :
   1 2 3 4
                     10
                        11 12
                               13 14 15 47
                                               48
                                                          55
              5
                8 9
                            81
                        80
   74 75 76 77 78 79
                                82
chain bonds :
                            11-46 12-40 13-52 17-18 19-20 19-21
                                                                 19-22
   2-6 3-8
           4 - 9
                5-37
                      10-38
ring bonds :
                     4-72 8-73 8-77 9-78 9-82 10-11 11-12 13-14 14-15 14-47
   1-2 1-5 3-4 3-72
   15-49 47-48 48-49 54-55 54-57 55-56 55-59 57-58 58-59 73-74 74-75 75-76 76-77
   78-79 79-80 80-81 81-82
exact/norm bonds :
   1-2 1-5 2-6 3-8 3-4 3-72 4-9 4-72
                                         5-37 10-11
                                                    10-38 11-12 11-46 12-40 13-14
   13-52 14-15 14-47 15-49 17-18 19-20
                                         19-21 19-22 47-48 48-49 54-55 54-57 55-56
   55-59 56-62 57-58 58-59
normalized bonds :
   8-73 8-77 9-78 9-82 73-74 74-75 75-76 76-77 78-79 79-80 80-81 81-82
isolated ring systems :
   containing 8 : 9 :
```

1:2 E exact RC ring/chain Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 37:CLASS 38:Atom 40:CLASS 43:Atom 46:CLASS 47:Atom 48:Atom 49:Atom 52:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 62:CLASS 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom Generic attributes : 6: Number of Hetero Atoms : 2 or more 38: Number of Hetero Atoms : 2 or more 43: : Unsaturated Saturation

Element Count :

52:

Node 6: Limited

: Unsaturated

N,N1

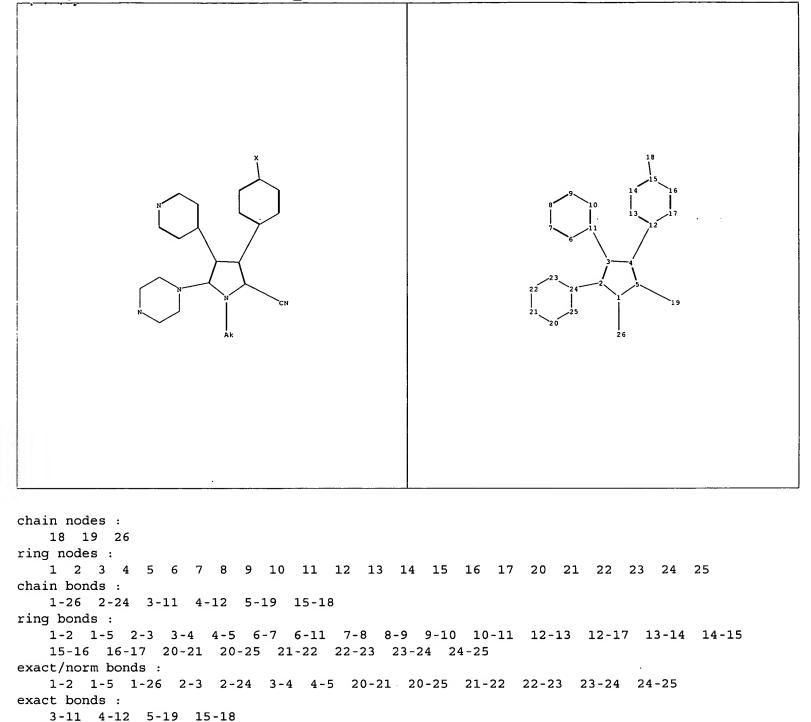
Saturation

Node 38: Limited

N,N1

Node 52: Limited

N,N1



Match level :

normalized bonds :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS

6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17